

Sylvanite (AgAuTe₄, *E1_b*) Structure: ABC4_mP12_13_e_a_2g-001

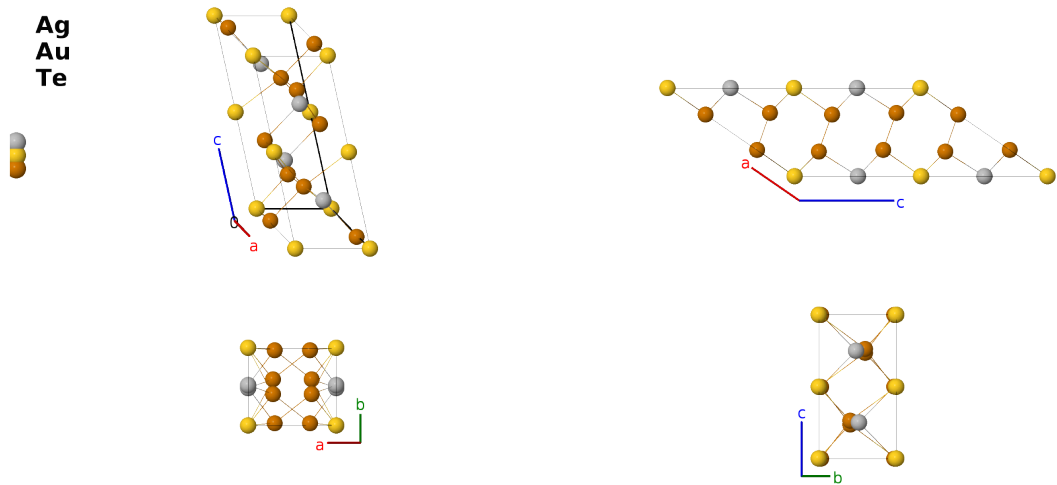
This structure previously used the label(s) `ABC4_mP12_13_e_a_2g`. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/5BWB>

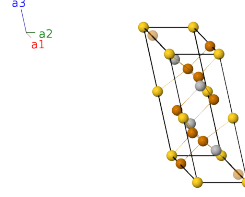
https://aflow.org/prototype-encyclopedia/ABC4_mP12_13_e_a_2g-001



Prototype	AgAuTe ₄
AFLOW prototype label	ABC4_mP12_13_e_a_2g-001
<i>Strukturbericht</i> designation	<i>E1_b</i>
Mineral name	sylvanite
ICSD	30874
CCDC	1605080
Pearson symbol	mP12
Space group number	13
Space group symbol	<i>P2/c</i>
AFLOW prototype command	<code>aflow --proto=ABC4_mP12_13_e_a_2g-001</code> <code>--params=a,b/a,c/a,β,y₂,x₃,y₃,z₃,x₄,y₄,z₄</code>

Simple Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= a \hat{\mathbf{x}} \\
\mathbf{a}_2 &= b \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(2a)	Au I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \cos \beta \hat{\mathbf{x}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(2a)	Au I
$\mathbf{B}_3$	$y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \cos \beta \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + \frac{1}{4} c \sin \beta \hat{\mathbf{z}}$	(2e)	Ag I
$\mathbf{B}_4$	$-y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \cos \beta \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + \frac{3}{4} c \sin \beta \hat{\mathbf{z}}$	(2e)	Ag I
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(a x_3 + c z_3 \cos \beta) \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \sin \beta \hat{\mathbf{z}}$	(4g)	Te I
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(a x_3 + c (z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	Te I
$\mathbf{B}_7$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(a x_3 + c z_3 \cos \beta) \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} - c z_3 \sin \beta \hat{\mathbf{z}}$	(4g)	Te I
$\mathbf{B}_8$	$x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(a x_3 + c (z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	Te I
$\mathbf{B}_9$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(a x_4 + c z_4 \cos \beta) \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \sin \beta \hat{\mathbf{z}}$	(4g)	Te II
$\mathbf{B}_{10}$	$-x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(a x_4 + c (z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	Te II
$\mathbf{B}_{11}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(a x_4 + c z_4 \cos \beta) \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} - c z_4 \sin \beta \hat{\mathbf{z}}$	(4g)	Te II
$\mathbf{B}_{12}$	$x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(a x_4 + c (z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4g)	Te II

References

- [1] F. Pertlik, *Kristallchemie natürlicher Telluride I: Verfeinerung der Kristallstruktur des Sylvanits, AuAgTe₄*, Tschermaks mineralogische und petrographische Mitteilungen **33**, 203–12 (1984), doi:10.1007/BF01081381.

Found in

- [1] P. Villars, *NaP Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database).

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